Chem 461/570 Physical Chemistry I Fall 2011

Professor	e-mail	Office Hour	Office
Eitan Geva	eitan@umich.edu	Friday 12:00-1:00 PM	2000D Chem.
GSI:			
Surma Talapatra	tsurma@umich.edu	Monday 12:00-1:00PM Wednesday 12:00-1:00PM	SLC alcove #4 SLC alcove #4

Website:

- Registered students will be granted access to the course website via https://ctools.umich.edu.
- Lecture notes, problem sets, answer keys, instructions and announcements from the instructor and GSI will be posted on the website.

Recommended textbook:

- Detailed lecture notes will be posted online and can serve as a substitute for a textbook.
- Consulting undergraduate physical chemistry books on the subject matter is encouraged but not required. Potentially useful texts include:
  1. "Quantum Chemistry" by Donald A. McQuarrie.
  2. "Physical Chemistry, A molecular approach" by Donald A. McQuarrie and John D. Simon (also covers thermodynamics, but the part about quantum mechanics is essentially the same as in text #1).
  3. "Quantum Chemistry" by Ira N. Levine.
  4. "Molecular Quantum Mechanics" by Peter Atkins and Ronald Friedman.
  5. Introduction to quantum mechanics in Chemistry" by Mark A. Ratner and George C. Schatz.
  6. "Elements of Quantum Mechanics" by Michael D. Fayer.
  7. "Introduction to Quantum Mechanics" by David J. Griffiths.

Class Schedule:

Lecture (Geva):	Section 200	MWF 11-12 PM	Room 1640 Chem
Discussion (GSI):	Section 201	Monday 4-5 PM	Room 1650 Chem
Discussion (GSI):	Section 202	Thursday 8-9 AM	Room 1632 Chem

Discussion sessions:

- **Attending the discussion sessions is required!**
- There will be no discussion sessions or office hours during the first week of classes (Sep. 6-9).
- There is no difference between the two discussion sessions.
- The discussion sessions will involve working out examples related to the material covered in the lecture with emphasis on the development of problem solving skills.

Exams:

Midterm Exam 1:	Tue.	October 11	6:00-8:00 PM	1640 Chem
Midterm Exam 2:	Tue.	November 22	6:00-8:00 PM	1640 Chem
Final Exam:	Mon.	December 19	1:30-3:30 PM	Location TBA

- You may bring **two** 8-1/2 by 11 inch formula sheets to mid-term exam 1**, four** formula sheets to mid-term exam 2, and six formula sheets to the final exam. You may write on both sides. You should also bring a **calculator** to the exams. In addition, you will be provides with sheets of physical constants and conversion factors and a periodic table similar to those posted in the course web site.

Grading:	Midterm Exam 1	100 pts.	
	Midterm Exam 2	250 pts.	(cumulative)
	Final Exam	350 pts.	(cumulative)
	6 Problem Sets	300 pts.	(50 pts. each)
	Total:	1000 pts	

Problem Sets:

Students are **required** to submit 6 problem sets. Each problem set is worth 50 points. **The problem sets will be posted on the web site**. The dates for posting and submission deadlines are given in the table below:

Problem set #	Date posted	Submission deadline
1	Sep. 7 2011	Sep. 23 2011
2	Sep. 23 2011	Oct. 7 2011
3	Oct. 7 2011	Oct. 24 2011
4	Oct. 24 2011	Nov. 7 2011
5	Nov. 7 2011	Nov. 18 2011
6	Nov. 18 2011	Dec. 9 2011

The problem sets are due by the end of the lecture on the indicated date.

- **Problem sets must be prepared legibly with work shown in an orderly and logical manner. The GSI may deduct points for problem sets that are messy or difficult to follow. Credit will not be given for numerical answers without worked solutions or for a correct answer if it is evident that your procedure is incorrect, unclear, or insufficient.**
- **Numerical answers must be given with correct units.**
- **Submission after the deadline will not be accepted (unless approved by the instructor in advance).**
- **Answer keys will be posted on the CTools site following the submission deadline.**

Demos:

Many of the interactive demos that will be used in class are available for free download at: http://demonstrations.wolfram.com/search.html?query=Eitan+Geva

List of topics:

1. The principles of classical physics.
2. The mathematical tools of quantum mechanics.
3. The postulates of quantum mechanics
4. Free particle and a particle in a box.
5. Approximate methods (the variational principle and time-independent perturbation theory).
6. Time-dependent perturbation theory and spectroscopy.
7. The harmonic oscillator and molecular vibrations.

8. Orbital angular momentum and molecular rotations.
9. The Hydrogen atom.
10. Spin angular momentum.
11. Multi-electron atoms (atomic orbital theory).
12. The chemical bond in diatomic molecules (molecular orbitals).
13. Chemical bonding in polyatomic molecules.